Effective Properties of Creeping Solids Undergoing Grain Boundary Sliding

GREGORY J. RODIN and MICHEL W. DIB

Texas Institute for Computational Mechanics, Department of Aerospace Engineering and Engineering Mechanics, The University of Texas at Austin, Austin, Texas 78712, USA

ABSTRACT

Grain boundary sliding is an important mode of deformation at elevated temperatures. It is central to nucleation and growth of grain boundary cavities. Sliding also often makes a substantial contribution to the total creep strain of the specimen. An attempt to calculate the stress enhancement factor in a statistical array of grains is undertaken. Simple geometrical characterization provides reasonable estimate.

KEYWORDS

Effective properties, creep, grain boundary sliding.

INTRODUCTION

Intergranular cavitation is one of the most important factors contributing to processes of creep deformation and fracture of polycrystalline materials (see, for example, Evans, 1984). Nucleation of grain boundary cavities requires high concentrations of normal stresses and is usually observed on boundaries with the normal aligned with the direction of the local maximum principal stress (Hayhurst, 1983). High stresses may emerge as the result of grain boundary sliding in the presence of hard second-phase particles. The particles serve as the stress concentrators while sliding is the consequence of relatively fast relaxation of intergranular shear stresses at elevated temperatures. On the macroscopic level we associate the above microscopic processes with damage accumulation and conventionally term the phenomenon as tertiary creep. For a variety of modern structures, tertiary creep may constitute a substantial part of service time and therefore further understanding of the mechanical behavior is important.

Although both grain boundary sliding and cavitation take place at the level of a grain diameter, it is important to realize that often by the time cavitation becomes active, sliding has been already fully developed. Under these circumstances the minimum creep rate or the onset of cavitation is measured in already damaged material. Therefore macroscopically-observed tertiary creep may constitute the difference between material with grain boundary sliding and cavitation, and material with sliding only.

The effect of grain boundary sliding on the macroscopic response has been considered by several authors. Crossman and Ashby (1975) and Gharemani (1980) analyze a two-dimensional array of hexagonal grains. Chen and Argon (1979) and Riedel (1984) model sliding boundaries by shear cracks. Beere (1982) calculated the effect of grain boundary sliding in cubic grains. Anderson and Rice (1985) make an important observation about the different nature of geometrical constraints in two- and three-dimensional arrays of grains. Evans (1984) and Riedel (1987) present comprehensive reviews of up-to-date experimental and theoretical information on the subject.

In this investigation we attempt to establish relationships between the additional compliance caused by grain boundary sliding and a geometrical structure of a statistical polycrystal.

BACKGROUND

We assume that under uniaxial tension the microscopically homogeneous material exhibits a power-law relation between the strain rate and the applied stress

$$\dot{\epsilon} = \dot{\epsilon}_0 \left(\frac{\sigma}{\sigma_0}\right)^n. \tag{1}$$

Material constants σ_0 and $\dot{\epsilon}_0$ denote the plastic deformation resistance and a reference minimum creep rate at room temperature (Brown and Ashby, 1980); n is a material exponent varying usually from three to eight. For an isotropic incompressible material, the three-dimensional analog of (1) defines the traceless strain rate tensor

$$\dot{\mathbf{E}} = \frac{3\dot{\epsilon}_0}{2\sigma_0} \left(\frac{\bar{\sigma}}{\sigma_0}\right)^{n-1} \mathbf{S}.\tag{2}$$

2

The Mises equivalent stress is

$$\tilde{\sigma} = \left(\frac{3}{2}\mathbf{S}\cdot\mathbf{S}\right)^{\frac{1}{2}},\tag{3}$$

and the stress deviator is given in terms of the Cauchy stress, T, by

$$\mathbf{S} = \mathbf{T} - \frac{1}{3} \left(tr \mathbf{T} \right) \mathbf{I}. \tag{4}$$

The second rank identity tensor is designated by I.

The above constitutive equations characterize the response in the absence of grain boundary sliding and we consider the entries in (1)-(4) being defined on the micro-

scopic level. Grain boundary sliding is neither associated with any preferred orientation nor produces opening displacements along the boundaries. Therefore the tensorial structure of (2)-(4) does not change and the changes are reflected by the one-dimensional equation

 $\dot{\epsilon} = \dot{\epsilon}_0 \left(f \frac{\sigma}{\sigma_0} \right)^a. \tag{5}$

Some authors "formally" call f the stress enhancement factor. This terminology is somewhat confusing because there is the actual enhancement of normal stresses on some of the grain boundaries. We consider the case of fully-developed grain boundary sliding with completely relaxed shear stresses along the boundaries. In this case the stress enhancement factor depends upon non-dimensional geometrical parameters and the material exponent.

The main geometrical measure of a microstructure is a grain size. Langdon's and Vastava's (1982) experiments on aluminum suggest that the creep strain rate increase due to sliding is approximately inversely proportional to a grain size. Let us examine this observation. We define the grain diameter d as the arithmetic mean of the intercepted length from a large number of random penetrations of a grain by a straight line (we use Underwood, 1970 as the reference on quantitative stereology). We assume that grains have planar convex faces. The total area of grain-boundaries, A, within a polycrystal of the volume V and the grain diameter d, is

$$A = \frac{2V}{d}. (6)$$

It would be tempting to conclude that for a fixed volume, materials with finer grains undergo more sliding because of the larger area available for sliding. This is not true as the stress enhancement factor can only depend upon non-dimensional parameters. The experimental evidence supporting the phenomenological observation of Langdon and Vastava (1982) is the presence of the local accommodation processes such as folds at the triple point junctions. For finer grains the relative importance of the folds increases as shown in Fig. 1 (Chang and Grant, 1956). Therefore the dependence of the stress enhancement factor should also include typical length scales of dislocational networks or grain boundary diffusion paths besides the grain diameter. We limit our analysis to cases of the large grains; or to the "small-scale" folds localized at the triple point junctions. Under this condition the grain diameter does not enter the formulation.

Anderson and Rice (1985) emphasize the importance of the topological nature of a microstructure. Grains within a polycrystal form a random complex geometrical structure. However, it has been observed (Underwood, 1970, page 243) that for a large variety of materials averaged topological properties remain within fairly tight bounds. The pentagonal dodecahedron and the truncated octahedron (Fig. 2) bound such diverse structures as Al-Sn grains, β -brass grains, bubbles and vegetable cells. The corresponding average number of edges per face are 5.0 and 5.143, number of faces per grain are 12 and 14, and number of vertices per grain are 20 and 24. The truncated octahedron is a space-filling polyhedra, while the pentagonal dodecahedron is not although it is topologically close to a large number of grains. The natural question

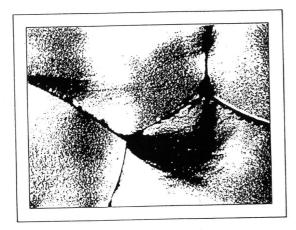


Fig. 1 Accommodating fold formation in Al-20%Zn (Chang and Grant, 1956).

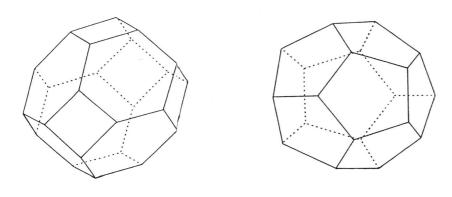


Fig. 2 Truncated octahedron (left) and pentagonal dodecahedron.

one could ask is whether such a primitive topological bounds can represent basis for physical modeling of grain boundary sliding in a random array of grains. Let us view the process of grain boundary sliding as a random distribution of planar convex surfaces with tangential discontinuities. This approach is exercized in the shear-crack models. Budiansky and O'Connell (1976) analyze arrays of random elliptical cracks and propose a single non-dimensional parameter characterization

$$\rho = \frac{1}{V} \sum_{i=1}^{i=N} \frac{A_i^2}{L_i}.$$
 (7)

In our case N is the number of grain boundaries of the area A_i and the perimeter L_i . The parameter is independent of the grain diameter and depends only upon the topological properties of a given array. An elementary calculation for a cube, truncated octahedron, and pentagonal dodecahedron gives

$$\rho_{cube} = 1.5 \quad \rho_{to} = 0.92 \quad \rho_{pd} = 0.92.$$

The equality (approximate) of the parameters for the two polyhedra is quite remarkable and may we suggest that for a random array of grains

$$\rho = \frac{1}{2}\rho_{to} = 0.46$$

It is reasonable to estimate the stress enchancement factor for a random array of grains as

$$f = f_{to}$$
.

Cubes are not representative of real grains but may serve as a test whether ρ is a good characterization of sliding in "an arbitrary" array.

THE STRESS ENHANCEMENT FACTOR

Beere (1982) reviews various models to calculate the stress enhancement factor and concludes that 1.1 < f < 2.1. He also gives an approximate analysis for the cubic array (Fig. 3). In his calculations the stress enhancement is 2.1 for n = 1 and 1.6 for n = 10.

Anderson and Rice (1985) analyze the array of the truncated octahedra. They employ a Ritz method using eight coordinate functions. They report f=1.65 and f=2.9 for n=1. The former is calculated for uniaxial tension normal to a family of the hexagonal faces while the latter is calculated for the square faces. We feel that the stress enhancement factors are too high and the array should not exhibit that degree of anisotropy.

We simulate the same problem within the environment of the finite element program ABAQUS. If the principal directions of the macroscopic strain tensor are normal to the square faces then it is sufficient to analyze only one eighth of the truncated octahedron (Fig. 4a). The boundary conditions on the inclined faces are rather complicated, and

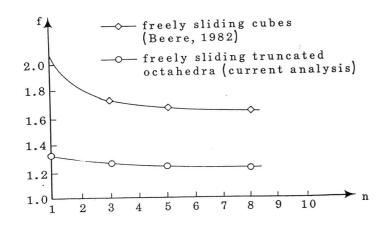


Fig. 3 Stress enhancement factor versus material exponent.

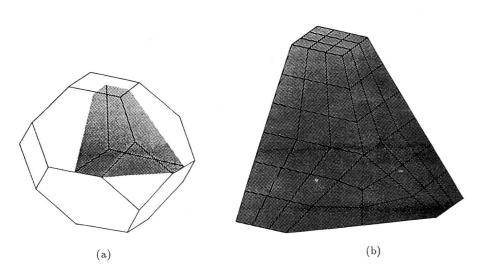


Fig. 4 Octant of truncated octahedron and its finite element model.

the detailed treatment can be found in Gharemani (1980) and Anderson and Rice (1985) appendices. The finite element mesh is shown in Fig. 4b. In the course of computations we find f = 1.31 for n = 1. The dependence of the stress enhancement factor on the material exponent is given on Fig. 3. Further analysis will be reported elsewhere.

DISCUSSION

Figure 3 displays the dependence of the stress enhancement factors upon the material exponent for infinite periodic arrays of cubes and truncated octahedra. Both curves exhibit the same tendency – slow descent with the increasing n. The most remarkable fact is that for n=1

$$f_{cube} = 1.90 \rho_{cube}$$
 and $f_{to} = 1.92 \rho_{to}$.

The correlation is not that good for n=8, and the corresponding numerical factors are 1.10 and 1.36. The deterioration may be explained in two ways. The simplest conclusion is that ρ by itself is a poor characterization grain boundary sliding in any array. We prefer more optimistic explanation that that the approximate analysis of Beere (1982) is less accurate for higher material exponents, n.

The principal conclusions are:

- The dependence of the stress enhancement factor on the grain diameter is primarily determined by networks of dislocations or diffusional processes and not by the area available for sliding.
- The geometrical constraints in fine-grain materials may be controlled by highly-localized accommodation in the form of folds. For larger grains we predict the stress enhancement factor

$$f = 2.8\rho$$

and in a statistical array of grains

$$f = 1.3$$

ACKNOWLEDGEMENTS

The research support of the National Science Foundations is gratefully appreciated.

REFERENCES

Anderson, P.M. and Rice, J.R. (1985). Acta Metall., 33, 409.

Beere, W. (1982). Metal Sci., 16, 223.

Budiansky, B. and O'Connell, R.J. (1976). Int. J. Solids Struct., 12, 81.

Brown A.M. and Ashby, M.F. (1980). Scripta Metall., 14, 1297.

Chang, H.C. and Grant, N.J. (1956). Trans. Am. Inst. Min. Metall Eng., 206, 544.

Chen, I.-W. and Argon, A.S. (1979). Acta Metall., 27, 785.

Crossman, F.W. and Ashby, M.F. (1975). Acta Metall., 23, 425.

Gharemani, F. (1980). Int. J. Solids Struct., 16, 847.

Evans, E.H. (1984). Mechanisms of Creep Fracture, Elsevier, New York.

Hayhurst, D.R. (1983). Engineering Approaches to High-Temperature Design, ed. Wilshire, B. and Owen, D.R.J., Swansea, U.K., 85.

Langdon, T.G. and Vastava, R.B. (1982). Mechanical Testing for Deformation Model Development, ASTM STP 765, ed. R.W. Rhode and J.C. Swearengen, American Society for Testing and Materials, 435.

Riedel, H. (1984). Acta Metall., 32, 313.

Riedel, H. (1987). Fracture at High Temperatures, Springer-Verlag, Berlin Heidelberg.

Underwood, E.E. (1970). Quantitative Stereology, Addison-Wesley, Reading, Massachusetts.